

# Spin dependent operators in correlated gaussian bases

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## Abstract

In their textbook, Suzuki and Varga [Y. Suzuki and K. Varga, *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems* (Springer, Berlin, 1998)] present the stochastic variational method with the correlated Gaussian basis in a very exhaustive way. The matrix elements for central potentials are put under a pleasant form but the elements for spin dependent operators, when treated, are given as very cumbersome expressions. In this paper, we find a lot of new formulae for those elements. Their expressions are given in terms of the same geometrical functions that appear in the case of central potentials. These functions get therefore a universal status; this property is very useful for numerical applications.

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## I. INTRODUCTION

There exist several different technical methods to solve the few-body problem with accuracy: Monte Carlo calculations [1], Faddeev and Yakubovsky treatments [2], hyperspherical formalism [3], expansion on various types of orthogonal [4], or non orthogonal bases [5]. Each technique shows specific advantages and drawbacks. Among others, the stochastic variational method is especially attractive. It relies on expansion of the wave function in term of gaussian type functions. The stochastic algorithm allows to consider very large bases with a minimum of variational effort. The drawback of this method is the non orthogonality of basis wave functions with the possibility of appearance of spurious states due to over-completeness; if this last inconvenience is overcome, using non orthogonal bases is not really a problem. The generalized eigenvalue problem arising in this case is well under control nowadays. The great advantage of using gaussian type functions is the rapid convergence and, above all, the possibility to compute the resulting matrix elements with analytical expressions most of time.

The stochastic variational method is described in full details in the remarkable textbook by Y. Suzuki and K. Varga [5], where most important and fundamental formulae are derived. This very complete work will be referred as SV throughout this paper, and all subsequent references can be found in it.

However a number of important formulae are missing and do not seem to appear in the literature. This was the case of the Fourier transform of the general corre-

lated Gaussian and its application to the matrix elements of the semi-relativistic kinetic energy operator. We presented such corresponding formulae in a recent paper [6], hereafter denoted SBM. In the same paper, we also propose new formulae for the matrix elements of the central potential, which are more efficient on the numerical point of view. Moreover, in the SV book, the matrix elements of spin-dependent operators are presented in a very cumbersome form.

Despite the fact that the calculations are more involved than the simpler central potential case, we have found a formulation that allows to express all these elements in an elegant and unified way. The aim of this paper is to present these new formulae and to convince the reader that complicated physical situations needing the use of central plus spin-dependent operators can be treated in a unified way based on universal functions. The gain of performance in a numerical treatment is very important.

We will derive expressions for the most general correlated gaussians (arbitrary number of particles  $N + 1$ , arbitrary angular momentum  $L$ , arbitrary radial  $K$  quantum number). We focus our interest on spin-dependent operators, but relegate in appendix some considerations on central potentials already given in SV and SBM, in order to achieve some self-consistency. Moreover, the non-natural parity states are very difficult to handle in correlated bases and, in the following, we just study natural parity (i.e spatial parity equal to  $(-1)^L$ ) states.

To calculate the same matrix elements, we will propose four different alternative expressions, with their own interests and drawbacks; this is very useful for numerical checks. A first approach sticks closely to the spirit of SV; the corresponding formulae exhibits nicely the symmetry properties. A second approach, proposed in SBM, gives formulae in which the symmetry properties are less transparent, but which are more efficient numerically. In both

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approaches, we give a formulation in terms of potential integrals  $J$  which depend on combinations of Hermite polynomials and make economical the final expression, and a formulation in terms of potential integrals  $\mathcal{F}$  which are universal and, most of the time, analytical.

The paper is organized as follows. We recall, in a first section, the description of the systems under consideration (intrinsic coordinates, definition of correlated Gaussians and their generating functions) and important definitions that are a link on all expressions presented here. The third section is devoted to the results concerning the spin-orbit operators, while the fourth section deals with tensor operators. In the appendixes, we give a number of important ingredients that should be used in the course of the various derivations of this work. Most of them are rather technical, but are also new relations that do not appear in the literature.

## II. THE SYSTEM UNDER CONSIDERATION

Since a lot of details concerning the system under consideration are already given in SBM, we recall here only a few things, referring the reader to this work for further information.

### A. Jacobi coordinates

Let us denote by  $N+1$  the number of particles ( $N \geq 1$ ); the position of particle  $i$ , of mass  $m_i$ , is  $\mathbf{r}_i$  in some frame, while the conjugate momentum is  $\mathbf{p}_i$ . In quantum mechanics and in position representation,  $\mathbf{r}_i$  and  $\mathbf{p}_i = -i\partial/\partial\mathbf{r}_i$  are operators in the Hilbert space of the states. The intrinsic properties of the system are described in terms of  $N$  Jacobi coordinates  $\mathbf{x}_i$  while the bulk properties are dependent of the center of mass coordinate  $\mathbf{R}$ .

In order to simplify the notations, let us introduce a “super-vector”  $\tilde{\mathbf{x}} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$  and write the coefficients of linear combinations as a “line (or column) matrix”, i.e  $\tilde{u} = (u_1, u_2, \dots, u_N)$ . This allows to shorten the expressions using the usual matrix operations. For example, a linear combination of Jacobi coordinates is denoted  $\tilde{u}\mathbf{x} = u_1\mathbf{x}_1 + u_2\mathbf{x}_2 + \dots u_N\mathbf{x}_N$ .  $A$  being a  $N \times N$  matrix, the expression  $A\mathbf{x}$  means the super vector  $(\sum_j A_{1j}\mathbf{x}_j, \sum_j A_{2j}\mathbf{x}_j, \dots, \sum_j A_{Nj}\mathbf{x}_j)$ . Lastly  $\tilde{\mathbf{x}} \cdot \mathbf{y}$  represents the scalar  $\mathbf{x}_1 \cdot \mathbf{y}_1 + \mathbf{x}_2 \cdot \mathbf{y}_2 + \dots + \mathbf{x}_N \cdot \mathbf{y}_N$  where the symbol  $\cdot$  deals with a spatial scalar product.

It is easy to show that both the operators  $\mathbf{r}_i - \mathbf{R}$  appearing in one-body potentials and the operators  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$  appearing in two-body potentials are combinations of Jacobi coordinates. Explicitly

$$\mathbf{r}_i - \mathbf{R} = \tilde{w}^{(i)}\mathbf{x}; \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j = \tilde{w}^{(ij)}\mathbf{x} \quad (1)$$

where the coefficients  $\tilde{w}^{(i)}$  and  $\tilde{w}^{(ij)}$  are mass dependent.

The conjugate momenta of the Jacobi coordinates are denoted  $\tilde{\boldsymbol{\pi}} = (\boldsymbol{\pi}_1, \boldsymbol{\pi}_2, \dots, \boldsymbol{\pi}_N)$  ( $\boldsymbol{\pi}_i = -i\partial/\partial\mathbf{x}_i$ ). In the

same way, both the operator  $\mathbf{p}_i$  (in the center of mass frame) appearing in one-body potentials and the operator  $\mathbf{p}_{ij} = (m_j\mathbf{p}_i - m_i\mathbf{p}_j)/(m_i + m_j)$  appearing in two-body potentials are combinations of Jacobi momenta. Explicitly

$$\mathbf{p}_i = \tilde{\zeta}^{(i)}\boldsymbol{\pi}; \mathbf{p}_{ij} = (m_j\mathbf{p}_i - m_i\mathbf{p}_j)/(m_i + m_j) = \tilde{\zeta}^{(ij)}\boldsymbol{\pi} \quad (2)$$

where, again, the coefficients  $\tilde{\zeta}^{(i)}$  and  $\tilde{\zeta}^{(ij)}$  are mass dependent.

In many variational methods, the wave function of the system is expanded on basis states as

$$|\Psi^{JM}\rangle = \sum_i C_i |\Psi_i^{JM}\rangle. \quad (3)$$

We forget about the colour, isospin and center of mass degrees of freedom and consider only space and spin degrees of freedom, since we are concerned only with spin-dependent potentials.  $JM$  are the total spin and magnetic quantum numbers for the system and  $|\Psi_i^{JM}\rangle$  are basis trial wave functions.

If some of the particles are identical, the basis states must be (anti)symmetrized with the help of a (anti)symmetrizer operator. In the stochastic variational method the resulting complications are not really a problem because correlated Gaussians with permuted coordinates are again correlated Gaussians with modified parameters and the spin functions can be handled with the well controlled Racah algebra. Thus the (anti)symmetrization complication essentially results only in adding linear combinations of wave functions of the same type. Thus, in order to simplify the presentation, we suppose basis wave functions that are not (anti)symmetrized.

In order to exploit fully the power of the formulation in terms of correlated Gaussians, one must adopt a coupling for angular momenta that is of type  $LS$  with a spatial wave function with total angular momentum  $L$  and a spin wave function of total spin  $S$ .

With this in mind, one writes one basis state as

$$|\Psi_i^{JM}\rangle = [|\Psi_{L_i}(1, \dots, N+1)\rangle |\chi_{S_i}(1, \dots, N+1)\rangle]_{JM}. \quad (4)$$

Concerning the spin function, there may occur several possibilities for the coupling to a spin  $S_i$ . In general, various intermediate couplings appear and are part of the quantum numbers necessary to label a basis state  $i$ . For example, in the three-body problem, one chooses the coupling  $[(s_1, s_2)_{S_{12i}} s_3]_{S_i}$  with only one intermediate quantum number  $S_{12i}$ . In contrast, in the four-body problem, one may choose the coupling  $[((s_1 s_2)_{S_{12i}} s_3)_{S_{123i}} s_4]_{S_i}$  with the two intermediate quantum numbers  $(S_{12i}, S_{123i})$  or the coupling  $[(s_1 s_2)_{S_{12i}} (s_3 s_4)_{S_{34i}}]_{S_i}$  with the two intermediate quantum numbers  $(S_{12i}, S_{34i})$ .

The spatial wave function is discussed more deeply in the next subsection.

## B. Correlated Gaussians

The so-called ‘‘correlated Gaussian’’ is a special form of space wave function which is widely used in the stochastic variational method. It is expressed in terms of the Jacobi coordinates. It has a number of advantages. In its most general version the convergence in terms of basis states is quite fast, and the way to deal with the angular momentum is in a form that allows to treat easily systems with arbitrary number of particles. Moreover, one can obtain most of the matrix elements under an analytical expression.

The argument of the exponential is a bilinear combination of the Jacobi coordinates:  $\sum_{i,j=1}^N A_{ij} \mathbf{x}_i \cdot \mathbf{x}_j = \tilde{\mathbf{x}} \cdot A \mathbf{x}$ . The matrix  $A$  must be symmetric ( $A = \tilde{A}$ ) and positive definite.

To deal with a non vanishing total angular momentum, one must introduce spherical harmonics somehow or other. The most elegant manner is to use a **single** solid harmonic  $\mathcal{Y}_{LM}(\mathbf{v}) = v^L Y_{LM}(\hat{\mathbf{v}})$ . To achieve some symmetry, and also to have more variational parameters at our disposal, the argument of the solid harmonic is the most general linear combination of the Jacobi coordinates  $\mathbf{v} = \sum_{i=1}^N u_i \mathbf{x}_i$ .

With those definitions, the most general correlated Gaussian is given by (note a slight difference with SV notations; their matrix  $A$  is twice ours and moreover  $N$  is the number of Jacobi coordinates while SV consider it as the number of particles)

$$\langle \mathbf{x} | \Psi_{KLM}(u, A) \rangle = f_{KLM}(u, A; \mathbf{x}) = \exp(-\tilde{\mathbf{x}} \cdot A \mathbf{x}) |\tilde{u} \mathbf{x}|^{2K} \mathcal{Y}_{LM}(\tilde{u} \mathbf{x}). \quad (5)$$

Thus, each basis state is described by  $N(N+3)/2$  free parameters ( $N(N+1)/2$  for the matrix  $A$  and  $N$  for the vector  $u$ ). This prescription (5) is only able to deal with natural parity states. The term  $|\tilde{u} \mathbf{x}|^{2K}$  is introduced for generality and to treat with more accuracy potentials with specific singular features. However, it complicates a lot the resulting expressions. It is often more convenient (except when the potential is so singular that the resulting integrals diverge) to keep in the calculation the correlated Gaussians restricted to  $K = 0$ , including more basis states to compensate a slower convergence.

## C. Matrix elements and generating functions

As explained in SV and SBM, the calculation of the matrix elements of some operator  $\hat{O}$  on the correlated gaussians, namely  $\langle \Psi_{K'L'M'}(u', A') | \hat{O} | \Psi_{KLM}(u, A) \rangle$  relies on the generating function technics.

Let us define the functions

$$g(\mathbf{s}, A; \mathbf{x}) = \exp(-\tilde{\mathbf{x}} \cdot A \mathbf{x} + \tilde{\mathbf{s}} \cdot \mathbf{x}) \quad (6)$$

where  $\mathbf{s}$  is an arbitrary super-vector,  $\tilde{\mathbf{s}} = (\mathbf{s}_1, \mathbf{s}_2, \dots, \mathbf{s}_N)$ .

The  $g$  functions are called the generating functions for the correlated Gaussians since one has

$$f_{KLM}(u, A; \mathbf{x}) = \frac{1}{B_{KL}} \times \int d\hat{\mathbf{e}} Y_{LM}(\hat{\mathbf{e}}) \left( \frac{\partial^{2K+L}}{\partial \lambda^{2K+L}} g(\lambda \mathbf{e} u, A; \mathbf{x}) \right)_{\lambda=0, |\mathbf{e}|=1} \quad (7)$$

where the geometrical coefficient  $B_{KL}$  is defined as

$$B_{KL} = \frac{4\pi(2K+L)!}{2^K K! (2K+2L+1)!!}. \quad (8)$$

In Eq. (7), the super-vector  $\mathbf{s} = \lambda \mathbf{e} u$  must be understood with all its components proportional to the same three vector  $\mathbf{e}$ , namely  $\mathbf{s}_i = \lambda u_i \mathbf{e}$ .

Using Eq. (7) in the expression of the searched matrix element leads to

$$\begin{aligned} & \langle \Psi_{K'L'M'}(u', A') | \hat{O} | \Psi_{KLM}(u, A) \rangle \\ &= \frac{1}{B_{K'L'} B_{KL}} \int d\hat{\mathbf{e}} d\hat{\mathbf{e}}' Y_{LM}(\hat{\mathbf{e}}) Y_{L'M'}^*(\hat{\mathbf{e}}') \\ & \times \left( \frac{\partial^{2K'+L'+2K+L}}{\partial \lambda'^{2K'+L'} \partial \lambda^{2K+L}} \langle \mathcal{O} \rangle \right)_{\lambda=\lambda'=0, |\mathbf{e}|=|\mathbf{e}'|=1}, \end{aligned} \quad (9)$$

with the matrix element between the generating functions

$$\langle \mathcal{O} \rangle = \langle g(\lambda' \mathbf{e}' u', A'; \mathbf{x}) | \hat{O} | g(\lambda \mathbf{e} u, A; \mathbf{x}) \rangle. \quad (10)$$

The matrix element that is left for computation is now between the generating functions, the form of which is much simpler.

Whatever the operator used in the Hamiltonian, it is scalar for rotations. Thus, the matrix elements do not depend on the magnetic quantum number  $M$ . Central potentials are spin independent; they have been treated extensively in BSM; some interesting formulae are gathered in appendix E. Here, we are mainly concerned with spin-orbit operators and tensor operators. Both are spin dependent.

## D. Universal functions

Generally, the expression for the matrix elements needs the introduction of several types of quantities:

- Dynamical quantities are functions of the explicit form of the operator  $\hat{O}$ . Any potential depends on some function of the Jacobi variables, for example for a two-body potential:  $V(|\mathbf{r}_i - \mathbf{r}_j|) = V(|\tilde{w}^{(ij)} \mathbf{x}|)$  (see (1)). In SV the dynamical resulting quantity is an integral of type

$$J(n, c) = \frac{1}{\sqrt{\pi}} \int_0^\infty V(x \sqrt{2/c}) e^{-x^2} Q_n(x) dx \quad (11)$$

where  $Q_n(x)$  is a specific function expressed in terms of Hermite polynomials. For the case of central potentials  $Q_n(x) = H_1(x)H_{2n+1}(x)/(2n+1)!$ .

In BSM, we proposed a new formulation for the matrix elements, which needs a more general integral

$$J(n, \alpha, c) = \frac{1}{\sqrt{\pi}} \int_0^\infty V\left(x\sqrt{2\frac{\alpha}{c}}\right) e^{-\alpha x^2} Q_n(x) dx, \quad (12)$$

with the same  $Q_n(x)$  function. Obviously  $J(n, c) = J(n, \alpha = 1, c)$ . The reason for appearance of such integrals is explained in Appendix B.

Although these functions are the most economical for a general presentation, they have several drawbacks: The function  $Q_n(x)$  depends on each type of potential considered (they are not identical for central, spin-orbit and tensor interactions), and the analytical expression of the  $J$  integrals, even for the simplest forms of  $V(x)$ , is not very simple. This is why, in BSM, we proposed also alternative expressions for the matrix elements in terms of a universal integral

$$\mathcal{F}_V(k, A) = \int_0^\infty V(u) u^k e^{-Au^2} du, \quad (13)$$

with integer value for  $k$ . Indeed, a lot of closed expressions exist for various forms of potentials  $V(u)$ .

- Pure geometrical quantities also appear in the formalism. For example, the coefficients  $B_{KL}$  are very common (see (8)). In the same way, the coefficients  $Z_l^\lambda$ , as defined by (C4), are also of some use.
- Lastly, geometrical functions depending on the various parameters of the problems were introduced both in SV and BSM. In SV, a very important function, appearing in the case of central potential, is defined by

$$F_{p,p',l}^n(u, u', v, w, w') = n! \sum_{m=0}^p \sum_{m'=0}^{p'} \frac{u^{p-m}}{(p-m)!} \frac{u'^{p'-m'}}{(p'-m')!} \times \frac{v^{l-n+m+m'}}{(l-n+m+m')!} \frac{w^{n+m-m'} w'^{n-m+m'}}{2^{m+m'} m! m'! (n-m-m')!} \quad (14)$$

(we have also the following constraints  $p+p'+l \geq n$  and  $n-l \leq m+m' \leq n$ ).

In BSM, another function of great importance is defined by

$$F_{n,k}^{K,K',L}(x, x', y, y') = n! \sum_{m=\max(k+L, n-K')}^{\min(n-k, K+L)} \frac{x^{K+L-m}}{(K+L-m)!} \times \frac{x'^{K'-n+m}}{(K'-n+m)!} \frac{y^{2m-L} y'^{2(n-m)+L}}{(m-k-L)!(n-k-m)!}. \quad (15)$$

The functions appearing in (14) and (15) are denoted with the same letter  $F$  but are not identical. They differ by the number of continuous arguments. The formulation in terms of  $F$  function (15) is more efficient numerically since the number of arguments is less (4 instead of 5) and the sum runs on a smaller number of indices (1 instead of 2). For central potential matrix elements, the  $F$  functions are associated to the  $J$  integrals.

Associated to the  $\mathcal{F}$  integrals, other functions, more complicated, are necessary. They are absent in SV, but have been given in BSM. In a first formulation, we need the following function

$$H_{n,k}^{K,K',L}(x, x', y) = \sum_{r=0}^{K+K'+L-n} (-1)^r \frac{(K+K'+L-r)! y^r}{(K+K'+L-n-r)!} G_{k,r}^{K,K',L}(x, x') \quad (16)$$

and

$$G_{k,r}^{K,K',L}(x, x') = \sum_{s=0}^{K-k} \sum_{s'=0}^{K'-k} \frac{x^s x'^{s'}}{s!(K-k-s)!s'!(K'-k-s')!} \times \frac{1}{(r-s-s')!(2k+L+s+s'-r)!} \quad (17)$$

while in a second formulation, it appears the following function

$$P_{n,k}^{K,K',L}(x, x', y, y', z) = \sum_{r=k+L}^{K+L} \frac{x^{K+L-r} x'^{K'+r-n} y^{2r-L} y'^{2(n-r)+L}}{(K+L-r)!(r-k-L)!} M_{n,k,r}^{K'}(z) \quad (18)$$

with

$$M_{n,k,r}^{K'}(z) = \sum_{s=\max(0, k+r-n)}^{K'+r-n} \frac{(s+n)!}{(K'+r-s-n)!(s+n-k-r)!} \frac{z^s}{s!}. \quad (19)$$

Here again, the second formulation (18) is numerically more efficient since the  $P$  function requires a summation on 2 indices while the  $H$  function requires 3 indices.

As we will see, all the quantities presented in this section – dynamical, purely geometrical factors or geometrical functions – have indeed a universal character and appear not only for central potentials, but also for any type of complicated potentials. This consequence is very beneficial on a numerical point of view since it allows to treat very different types of potentials with the same basic ingredients, which can be computed once and for all.

### III. SPIN-ORBIT POTENTIALS

In this section, we discuss about the spin-orbit potentials. Schematically, we have three types of spin-orbit potentials.

- One-body spin-orbit potential where the form of the operator for the particle  $i$  is given by (in the center of mass frame for the system)

$$V_i = V(|\mathbf{r}_i|) \mathbf{L}_i \cdot \mathbf{s}_i \quad (20)$$

where  $\mathbf{s}_i$  is the spin of the particle located at  $\mathbf{r}_i$ , with an angular momentum  $\mathbf{L}_i = \mathbf{r}_i \times \mathbf{p}_i$ , relative to the center of mass. Expressed in terms of Jacobi coordinates, it writes

$$V_i = V(|\tilde{w}^{(i)} \mathbf{x}|)(\tilde{w}^{(i)} \mathbf{x} \times \tilde{\zeta}^{(i)} \boldsymbol{\pi}) \cdot \mathbf{s}_i. \quad (21)$$

This kind of potential appears for instance as a relativistic correction of a flux tube model for hadron confining potential [8].

- What is called usually “spin-orbit” potential is the two-body symmetric spin-orbit potential, whose form is

$$V_{ij} = V(|\mathbf{r}_i - \mathbf{r}_j|) \mathbf{L}_{ij} \cdot \mathbf{S}_{ij} \quad (22)$$

where  $\mathbf{S}_{ij} = \mathbf{s}_i + \mathbf{s}_j$  is the total spin of the pair ( $i - j$ ), while  $\mathbf{L}_{ij} = \mathbf{r}_{ij} \times \mathbf{p}_{ij}$  is the angular momentum of the pair in its center of mass frame. Expressed in terms of Jacobi coordinates, it writes

$$V_{ij} = V(|\tilde{w}^{(ij)} \mathbf{x}|)(\tilde{w}^{(ij)} \mathbf{x} \times \tilde{\zeta}^{(ij)} \boldsymbol{\pi}) \cdot \mathbf{S}_{ij}. \quad (23)$$

This form of potential is traditional as a relativistic correction of one-photon, one-boson or one-gluon exchange potentials.

- Sometimes, it is necessary to introduce the two-body antisymmetric spin-orbit potential, defined by

$$V_{ij} = V(|\mathbf{r}_i - \mathbf{r}_j|) \mathbf{L}_{ij} \cdot \boldsymbol{\Delta}_{ij} \quad (24)$$

and which is very similar to (23) but with the spin operator  $\boldsymbol{\Delta}_{ij} = \mathbf{s}_i - \mathbf{s}_j$ . Expressed in terms of Jacobi coordinates, it writes

$$V_{ij} = V(|\tilde{w}^{(ij)} \mathbf{x}|)(\tilde{w}^{(ij)} \mathbf{x} \times \tilde{\zeta}^{(ij)} \boldsymbol{\pi}) \cdot \boldsymbol{\Delta}_{ij}. \quad (25)$$

This potential is also a relativistic correction of one-photon, one-boson or one-gluon exchange potentials. However, being proportional to  $1/m_i^2 - 1/m_j^2$ , it has no effect in the case of identical particles.

In order to simplify the notation let us note any of these potentials as  $V \mathcal{L} \cdot \mathcal{S}$  with obvious identification.  $\mathcal{L}$  and  $\mathcal{S}$  being vector operators, the matrix elements of the potential are obtained with help of Wigner-Eckart (WE)

formalism. Using (D2), one has generally the matrix element

$$\begin{aligned} \langle \Psi'^{J'M'} | V \mathcal{L} \cdot \mathcal{S} | \Psi^{JM} \rangle &= \delta_{JJ'} \delta_{MM'} (-1)^{J+S'+L} \\ &\times \left\{ \begin{matrix} L' & 1 & L \\ S & J & S' \end{matrix} \right\} \langle \Psi'^{K'L'} | V \mathcal{L} | \Psi^{KL} \rangle \langle \chi_{S'} | \mathcal{S} | \chi_S \rangle. \end{aligned} \quad (26)$$

The spin reduced element  $\langle \chi_{S'} | \mathcal{S} | \chi_S \rangle$  depends not only on the number  $N + 1$  of particles, but also on the type of coupling; it can be calculated specifically for each type of wave function. In any case, a closed (but somewhat complicated) formula is obtained with successive applications of WE theorem. An example is presented for the 3-body problem in Appendix D.

In this section, we are mainly concerned with the space matrix element. The prototype for the operator is

$$V = V(|\tilde{w} \mathbf{x}|)(\tilde{w} \mathbf{x} \times \tilde{\zeta} \boldsymbol{\pi}), \quad (27)$$

the parameters  $w, \zeta$  being  $w^{(i)}, \zeta^{(i)}$  for one-body operators and  $w^{(ij)}, \zeta^{(ij)}$  for two-body operators.

The starting point for the calculus is based on

$$\begin{aligned} \langle \Psi'^{K'L'} | V(|\tilde{w} \mathbf{x}|)(\tilde{w} \mathbf{x} \times \tilde{\zeta} \boldsymbol{\pi}) | \Psi^{KL} \rangle &= \int dr V(r) \\ \langle \Psi'^{K'L'} | \delta(|\tilde{w} \mathbf{x}| - r)(\tilde{w} \mathbf{x} \times \tilde{\zeta} \boldsymbol{\pi}) | \Psi^{KL} \rangle. \end{aligned} \quad (28)$$

The reduced matrix element in the integral is calculated with the help of the generating functions (see (9)) and with the expression (A5).

To simplify the notations, let us introduce the following notations (we stick as close as possible to the notations adopted in SV and SBM). First, with  $B = A + A'$ , one needs,

$$q = \frac{1}{4} \tilde{w} B^{-1} u; \quad q' = \frac{1}{4} \tilde{w}' B^{-1} u'; \quad \rho = \frac{1}{2} \tilde{w}' B^{-1} u. \quad (29)$$

Those scalar quantities are present in the term  $\mathcal{M}_0$  (see (A2)) and, as such, occur in the expression for the overlap and non relativistic kinetic energy matrix elements. Second, one must introduce

$$\begin{aligned} \gamma &= \frac{\tilde{w} B^{-1} u}{\tilde{w} B^{-1} w}; \quad \gamma' = \frac{\tilde{w} B^{-1} u'}{\tilde{w} B^{-1} w'}; \\ c &= \frac{2}{\tilde{w} B^{-1} w}; \quad z = \frac{1}{2} \tilde{w}' B^{-1} v. \end{aligned} \quad (30)$$

In addition to  $q, q', \rho$ , the scalars  $c, \gamma, \gamma'$  and the vector  $\mathbf{z}$  occur in the calculation of the matrix elements for central potentials. Lastly, the quantities

$$\eta = \tilde{\zeta} A' B^{-1} u; \quad \eta' = \tilde{\zeta} A B^{-1} u' \quad (31)$$

are scalars specific to spin-orbit potentials.

With those definitions, it is easy to show the equalities

$$\begin{aligned} c \mathbf{z} &= \gamma \lambda \mathbf{e} + \gamma' \lambda' \mathbf{e}' \\ \tilde{\zeta} \mathbf{y} &= \lambda \eta \mathbf{e} - \lambda' \eta' \mathbf{e}' \end{aligned} \quad (32)$$

so that (do not forget that  $|\mathbf{e}| = 1 = |\mathbf{e}'|$ )

$$\begin{aligned} c^2 z^2 &= \gamma^2 \lambda^2 + \gamma'^2 \lambda'^2 + 2\gamma\gamma'\lambda\lambda' \mathbf{e} \cdot \mathbf{e}' \quad (33) \\ \tilde{w} B^{-1} \mathbf{v} \times \tilde{\zeta} \mathbf{y} &= -\frac{2}{c}(\gamma\eta' + \gamma'\eta)\lambda\lambda' \mathbf{e} \times \mathbf{e}'. \end{aligned}$$

Let us focus on the term depending on  $\lambda, \lambda', \mathbf{e}, \mathbf{e}'$  since we must derive and integrate it. This term writes explicitly

$$e^{q\lambda^2 + q'\lambda'^2 + \rho\lambda\lambda' \mathbf{e} \cdot \mathbf{e}'} \frac{i_1(crz)}{z} e^{-cz^2/2} \lambda\lambda' [i(\mathbf{e} \times \mathbf{e}')]. \quad (34)$$

At this stage one can follow two roads:

- the road chosen by SV which leads to expressions in which the symmetry properties are very simple, but less efficient numerically;
- the road proposed by SBM whose symmetry properties are less transparent but more efficient numerically.

In order to give interesting and alternative expressions (very useful for numerical checks), let us present these two roads.

In the first road, the first exponential (coming from the  $\mathcal{M}_0$  quantity) is expanded in series of its arguments, while the  $z$ -depending functions are expressed in series of  $z^2$  with help of formula (B6). Lastly, the corresponding powers of  $z^2$  are expanded in powers of  $\lambda, \lambda', \mathbf{e} \cdot \mathbf{e}'$  using (33). All powers of  $\lambda, \lambda'$  and  $\mathbf{e} \cdot \mathbf{e}'$  are then gathered. The integration over  $\mathbf{e}$  and  $\mathbf{e}'$  is performed using the expression given by (C10) (forget about the Clebsch-Gordan coefficient since it cancels taking the reduced matrix element). The derivation on variable  $\lambda$  is easily obtained remarking that  $\partial\lambda^n/\partial\lambda^{2K+L}|_{\lambda=0} = (2K+L)! \delta_{2K+L,n}$  and an analogous relation for the derivation on variable  $\lambda'$ . The rest of the calculation is just matter of lengthy but straightforward algebra. It is very interesting to note that, as it was the case for central potential, the universal function  $F_{p,p',l}^n$  (as given by (14)) also occurs in the case of spin-orbit potentials. The final result for the reduced space matrix element writes explicitly

$$\begin{aligned} \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{KL} \rangle &= \delta_{L,L'} (\gamma\eta' + \gamma'\eta) \\ &\times \sqrt{L(L+1)(2L+1)} \frac{(2K+L)!(2K'+L')!}{B_{KL}B_{K'L'}} \\ &\times \left( \frac{\pi^N}{\det B} \right)^{3/2} \sum_{n=0}^{K+K'+L-1} \frac{1}{c^{n+1}} J(n, c) \\ &\times \sum_{k=0}^{\min(K,K')} \frac{B_{kL}}{2k+L} F_{K-k, K'-k, 2k+L-1}^n(q, q', \rho, \gamma, \gamma') \end{aligned} \quad (35)$$

where the dynamical integral  $J(n, c)$  is given by (11) with the value of the  $Q_n(x)$  function

$$Q_n(x) = H_1(x) K_n^{(1)}(x) \quad (36)$$

and the function  $K_n^{(1)}(x)$  defined by (B4) with the special value  $l = 1$ .

The very important peculiar case  $K = K' = 0$  leads to substantial simplifications since Eq. (35) reduces to

$$\begin{aligned} \langle \Psi'^{0L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{0L} \rangle &= \delta_{L,L'} \\ \sqrt{L(L+1)(2L+1)} \left( \frac{\eta}{\gamma} + \frac{\eta'}{\gamma'} \right) (L-1)! \mathcal{N}_L &\quad (37) \\ \sum_{n=0}^{L-1} \frac{1}{(L-1-n)!} J(n, c) \left( \frac{\gamma\gamma'}{\rho c} \right)^{n+1} \end{aligned}$$

One sees that the expression is very similar to that corresponding to central potentials (in particular the overlap  $\mathcal{N}_L$ , defined in (E2), factorizes), and this is very interesting for numerical efficiency.

In practice, it is better to use the  $\mathcal{F}$  dynamical integrals instead of the  $J$  dynamical integrals. In order to do that, the first step is to get the series expansion of the  $Q_n(x)$  function:

$$Q_n(x) = (-1)^n \sum_{r=0}^n (-1)^r \frac{(r+1)(2x)^{2r+4}}{(2r+3)!(n-r)!}. \quad (38)$$

This expression allows to provide the link between both types of dynamical integrals

$$\begin{aligned} J(n, c) &= (-1)^n \sqrt{\frac{c}{2\pi}} \\ &\times \sum_{r=0}^n (-1)^r \frac{(r+1)}{(2r+3)!(n-r)!} (2c)^{r+2} \mathcal{F}_V(2r+4, c/2). \end{aligned} \quad (39)$$

Using this expression in (35), and rearranging the summations it is possible to write the searched matrix element in term of the  $\mathcal{F}$  integrals:

$$\begin{aligned} \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{KL} \rangle &= \delta_{L,L'} \\ &\times \sqrt{\frac{L(L+1)(2L+1)}{\pi}} \frac{(2K+L)!(2K'+L')!}{2^{K+K'} B_{KL} B_{K'L'}} \left( \frac{2c\pi^N}{\det B} \right)^{3/2} \\ &\times \gamma^{2K+L} \gamma'^{2K'+L'} \left( \frac{\eta}{\gamma} + \frac{\eta'}{\gamma'} \right) \left( -\frac{1}{c} \right)^{K+K'+L-1} \\ &\times \sum_{n=0}^{K+K'+L-1} \frac{(n+1)}{(2n+3)!} (-2c)^n \mathcal{F}_V(2n+4, c/2) \\ &\times \sum_{k=0}^{\min(K,K')} 4^k \frac{B_{kL}}{2k+L} H_{n,k}^{K,K',L-1} \left( \frac{2q\gamma'}{\rho\gamma}, \frac{2q'\gamma'}{\rho\gamma'}, \frac{\rho c}{\gamma\gamma'} \right). \end{aligned} \quad (40)$$

Here again, it is very pleasant to ascertain that it appears in this expression the same geometrical  $H$  function (16) as in the central potential expression (compare to (E9)).

For the peculiar important case  $K = K' = 0$ , the matrix element has a much simpler form:

$$\begin{aligned} \langle \Psi'^{0L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{0L} \rangle &= \delta_{L,L'} (L-1)! \mathcal{N}_L \\ &\times \sqrt{\frac{L(L+1)(2L+1)}{8\pi c}} \left( \frac{\eta}{\gamma} + \frac{\eta'}{\gamma'} \right) \sum_{n=0}^{L-1} \mathcal{F}_V(2n+4, c/2) \\ &\times \frac{(n+1)(2c)^{n+3}}{(2n+3)!(L-1-n)!} \left( \frac{\gamma\gamma'}{\rho c} \right)^{n+1} \left( 1 - \frac{\gamma\gamma'}{\rho c} \right)^{L-1-n}. \end{aligned} \quad (41)$$

This expression is very similar to (37) (at least as simple) but has the big advantage to be given in terms of  $\mathcal{F}$  integrals instead of the more complicated  $J$  integrals; thus this expression is much more suited for a numerical code.

In the second road, we take opportunity of the link between  $\mathbf{e} \cdot \mathbf{e}'$  and  $z^2$  given in eq. (33) to transform the first exponential in (34) under a form containing  $z^2$  instead of  $\mathbf{e} \cdot \mathbf{e}'$ . The part depending on  $z^2$  is then gathered with the second exponential in (34). This trick allows to gain one series expansion in the development of (34) and, thus, a summation index less than in the former treatment. Indeed, instead of (34), our expansion is based on the alternative form

$$e^{\bar{q}\lambda^2 + \bar{q}'\lambda'^2} \frac{i_1(crz)}{z} e^{-\alpha cz^2/2} \lambda\lambda' [i(\mathbf{e} \times \mathbf{e}')]. \quad (42)$$

with introduction of new parameters

$$\bar{q} = q - \frac{\rho\gamma}{2\gamma'}; \quad \bar{q}' = q' - \frac{\rho\gamma'}{2\gamma}; \quad \alpha = 1 - \frac{\rho c}{\gamma\gamma'}. \quad (43)$$

The rest of the derivation is quite similar to what was done previously.

Thus we have a new expression for the matrix element

$$\begin{aligned} \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{KL} \rangle &= \delta_{L,L'} (\gamma\eta' + \gamma'\eta) \\ &\times \sqrt{\frac{L(L+1)(2L+1)}{4\pi}} \frac{(2K+L)!(2K'+L')!}{B_{KL}B_{K'L'}} \left( \frac{\alpha\pi^N}{\det B} \right)^{3/2} \\ &\times \sum_{n=0}^{K+K'+L-1} \left( \frac{\alpha}{2c} \right)^{n+1} J(n, \alpha, c) \\ &\times \sum_{k=0}^{\min(K,K')} 2^{2k+L} \frac{B_{kL}}{(2k+L)!} F_{n,k}^{K,K',L-1}(\bar{q}, \bar{q}', \gamma, \gamma'). \end{aligned} \quad (44)$$

where the integral  $J(n, \alpha, c)$  is defined by (12) with the same function  $Q_n(x)$  as before (36).

Once more, the universal function  $F$ , given by (15), appears naturally. As explained, this expression is better suited for numerical calculation as compared to the analogous formulation (35).

The peculiar case  $K = K' = 0$  is particularly simple

$$\begin{aligned} \langle \Psi'^{0L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{0L} \rangle &= \delta_{L,L'} \\ &\times \sqrt{\frac{L(L+1)(2L+1)}{4\pi}} \left( \frac{\eta}{\gamma} + \frac{\eta'}{\gamma'} \right) (L-1)! \mathcal{N}_L \\ &\times \alpha^{3/2} \left( \frac{\alpha}{1-\alpha} \right)^L J(L-1, \alpha, c). \end{aligned} \quad (45)$$

Since the integral  $J(L-1, \alpha, c)$  needs essentially the same numerical effort than the integral  $J(n, c)$ , it is obvious that the new formula (45) is much efficient than its analog (37); it is a closed analytical expression without any summation!

Let us close this section by giving new expressions in terms of the dynamical  $\mathcal{F}$  integrals. Always with the help of (38), the link between the  $J$  integrals and the  $\mathcal{F}$  integrals is given by

$$\begin{aligned} J(n, \alpha, c) &= (-1)^n \sqrt{\frac{c}{2\pi\alpha}} \\ &\times \sum_{r=0}^n \frac{(-1)^r (r+1)}{(2r+3)!(n-r)!} \left( \frac{2c}{\alpha} \right)^{r+2} \mathcal{F}_V(2r+4, c/2). \end{aligned} \quad (46)$$

The final expression for the general matrix element looks similar to

$$\begin{aligned} \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|)(\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) || \Psi^{KL} \rangle &= \delta_{L,L'} (\gamma\eta' + \gamma'\eta) \\ &\times \sqrt{\frac{L(L+1)(2L+1)}{4\pi}} \frac{(2K+L)!(2K'+L')!}{B_{KL}B_{K'L'}} \left( \frac{2c\pi^N}{\det B} \right)^{3/2} \\ &\times \sum_{n=0}^{K+K'+L-1} \frac{(n+1)}{(2n+3)!} \mathcal{F}_V(2n+4, c/2) \\ &\times \sum_{k=0}^{\min(K,K')} 2^{2k+L} \frac{B_{kL}}{(2k+L)!} P_{n,k}^{K,K',L-1} \left( \bar{q}, \bar{q}', \gamma, \gamma', \frac{-\alpha\gamma'^2}{2c\bar{q}'} \right). \end{aligned} \quad (47)$$

The  $P$  function has been defined in (18).

Application of this formula to the special case  $K = K' = 0$  does not bring anything new since it reduces to the one already got previously (see (41))

#### IV. TENSOR FORCE

In few and many-body systems, the tensor force is of common use. We discuss here the two-body tensor force  $V^{(T)} = \sum_{i \leq j} V_{ij}^{(T)}(\mathbf{r}_{ij})$ .

The form of this potential for the  $(i-j)$  pair is traditional

$$V_{ij}^{(T)}(\mathbf{r}_{ij}) = V(|\mathbf{r}_{ij}|) \hat{S}_{ij}; \quad \hat{S}_{ij} = 3(\mathbf{s}_i \cdot \hat{\mathbf{r}}_{ij})(\mathbf{s}_j \cdot \hat{\mathbf{r}}_{ij}) - \mathbf{s}_i \cdot \mathbf{s}_j. \quad (48)$$

Very often we find an alternative form for the tensor operator namely

$$\hat{S}_{ij} = 3(\mathbf{S}_{ij} \cdot \hat{\mathbf{r}}_{ij})^2 - \mathbf{S}_{ij}^2. \quad (49)$$

where the total spin of the pair  $\mathbf{S}_{ij} = \mathbf{s}_i + \mathbf{s}_j$  enters the game. Strictly speaking both forms are fully equivalent (up to a factor 2) only for spin 1/2 particles. However, in deriving the interaction between particles it appears, in addition to the form (48), terms depending on  $(\mathbf{s}_i \cdot \hat{\mathbf{r}}_{ij})^2$  and  $(\mathbf{s}_j \cdot \hat{\mathbf{r}}_{ij})^2$  which can be absorbed in the former expression to give a term similar to (49) (up to uninteresting constants). A more detailed discussion about these forms for the tensor force can be found in ref. [9]. Thus, both forms can be considered as equivalent and are of common use.

To treat easily the tensor force, it is better to express it in a form that splits the space and spin degrees of freedom. It is well known that this operator can be recast under form (the dot means the scalar product, while the bracket means the coupling to 0 angular momentum).

$$\begin{aligned} \hat{S}_{ij} &= \sqrt{\frac{24\pi}{5}} (Y_2(\hat{\mathbf{r}}_{ij}) \cdot \mathbf{S}_{ij}) \\ &= \sqrt{24\pi} [Y_2(\hat{\mathbf{r}}_{ij}) \otimes \mathbf{S}_{ij}]_{00} \end{aligned} \quad (50)$$

with one of the alternative expression

$$\mathbf{S}_{ij} = (\mathbf{s}_i \otimes \mathbf{s}_j)_2 \quad \text{or} \quad \mathbf{S}_{ij} = (\mathbf{S}_{ij} \otimes \mathbf{S}_{ij})_2. \quad (51)$$

Using again (D2), one has

$$\begin{aligned} \langle \Psi'^{J'M'} | V_{ij}^{(T)} | \Psi^{JM} \rangle &= \delta_{JJ'} \delta_{MM'} (-1)^{J+S'+L} \\ &\times \sqrt{\frac{24\pi}{5}} \left\{ \begin{matrix} L' & 2 & L \\ S & J & S' \end{matrix} \right\} \langle \chi_{S'} | \mathbf{S}_{ij} | \chi_S \rangle \\ &\times \langle \Psi'^{K'L'} | V(|\mathbf{r}_{ij}|) Y_2(\hat{\mathbf{r}}_{ij}) | \Psi^{KL} \rangle. \end{aligned} \quad (52)$$

The spin matrix elements  $\langle \chi_{S'} | \mathbf{S}_{ij} | \chi_S \rangle$  must be calculated separately for each type of coupling for a given system. Anyhow, this calculation can always be performed by successive application of Wigner-Eckart theorem and with the help of (D2). The corresponding formulae for the three-body systems are presented in Appendix D (see (D9-D12)).

In the rest of this section, we focus on the space matrix element. Because of (1), we are concerned with the matrix element

$$\begin{aligned} \langle \Psi'^{K'L'} | V(|\tilde{\mathbf{w}}\mathbf{x}|) Y_2(\widehat{\tilde{\mathbf{w}}\mathbf{x}}) | \Psi^{KL} \rangle &= \\ \int dr V(r) \langle \Psi'^{K'L'} | \delta(|\tilde{\mathbf{w}}\mathbf{x}| - r) Y_2(\widehat{\tilde{\mathbf{w}}\mathbf{x}}) | \Psi^{KL} \rangle. \end{aligned} \quad (53)$$

The derivation is quite similar to the one presented in the case of spin-orbit potential and we do not repeat the arguments. Let us just point out a trick that was used; the term  $Y_{2\mu}(\widehat{2\mathbf{z}})$  that appears can be transformed to  $Y_{2\mu}(\hat{\mathbf{z}}) = \mathcal{Y}_{2\mu}(c\mathbf{z})/(c^2 z^2)$ . With the expression (32) for

$c\mathbf{z}$ , and the values (C8) for the integral on the variables  $\mathbf{e}, \mathbf{e}'$ , the rest of the calculation is straightforward.

Let us give first the matrix element obtained by “the first road”. The most general expression is

$$\begin{aligned} \langle \Psi'^{K'L'} | V(|\tilde{\mathbf{w}}\mathbf{x}|) Y_2(\widehat{\tilde{\mathbf{w}}\mathbf{x}}) | \Psi^{KL} \rangle &= \delta_{L\pm 2 \text{ or } L, L'} \\ &\times \sqrt{\frac{5}{4\pi}} \frac{(2K+L)!(2K'+L')!}{B_{KL} B_{K'L'}} \left( \frac{\pi^N}{\det B} \right)^{3/2} \gamma \gamma' \\ &\times \sqrt{\frac{L_m(L_m+1)}{2L_m+1}} \sum_{n=0}^{K+K'+L_m-1} \frac{1}{c^{n+1}} J(n, c) \\ &\times \sum_{l=0}^2 \sum_{k=0}^{\min(\bar{K}_l, \bar{K}'_l)} \mathcal{A}_{kl}^{L, L'}(\gamma, \gamma') F_{\bar{K}_l-k, \bar{K}'_l-k, 2k+\bar{L}_l}^n(q, q', \rho, \gamma, \gamma') \end{aligned} \quad (54)$$

where the dynamical integral  $J(n, c)$  is given by (11) with the value of the  $Q_n(x)$  function

$$Q_n(x) = \frac{K_n^{(2)}(x)}{x} \quad (55)$$

and the function  $K_n^{(l)}(x)$  defined by (B4) with the special value  $l = 2$ . The geometrical coefficients  $\mathcal{A}$  are given by

$$\mathcal{A}_{kl}^{L, L\pm 2}(\gamma, \gamma') = \sqrt{\frac{3}{2}} 2^{\bar{l}} (R_{\pm})^{l-1} B_{k(L_i+l)}; \quad (56a)$$

$$\begin{aligned} \mathcal{A}_{kl}^{L, L}(\gamma, \gamma') &= -\frac{2L+1}{\sqrt{(2L-1)(2L+3)}} (R_+)^{l-1} \\ &\times B_{kL} \frac{(4k+2L+2+\bar{l})}{2^{1-\bar{l}}(2k+L+1-\bar{l})}; \end{aligned} \quad (56b)$$

$$R_+ = \gamma/\gamma' \quad ; \quad R_- = \gamma'/\gamma;$$

where new quantities are introduced below

$$\begin{aligned} \bar{K}_l &= K-l; \quad \bar{K}'_l = K'; \quad \bar{L}_l = L+l \quad \text{for} \quad L' = L+2 \\ \bar{K}_l &= K-f_l; \quad \bar{K}'_l = K'-f'_l; \quad \bar{L}_l = L-\bar{l} \quad \text{for} \quad L' = L \quad (57) \\ \bar{K}_l &= K; \quad \bar{K}'_l = K'-l; \quad \bar{L}_l = L-2+l \quad \text{for} \quad L' = L-2 \end{aligned}$$

and

$$L_m = (L+L')/2; \quad L_i = \min(L, L'); \quad \bar{l} = \text{mod}(l, 2); \quad (58)$$

$$f_l = (l-\bar{l})/2; \quad f'_l = (2-l-\bar{l})/2. \quad (59)$$

For the special case  $K = K' = 0$  the corresponding expressions are much simpler

$$\begin{aligned} \langle \Psi'^{0L'} | V(|\tilde{\mathbf{w}}\mathbf{x}|) Y_2(\widehat{\tilde{\mathbf{w}}\mathbf{x}}) | \Psi^{0L} \rangle &= \delta_{L\pm 2 \text{ or } L, L'} \\ &\times \sqrt{\frac{5}{4\pi}} \sqrt{L_m(L_m+1)} \mathcal{N}_{L_m}(L_m-1)! \mathcal{D}^{L, L'}(\gamma, \gamma') \\ &\times \sum_{n=0}^{L_m-1} \frac{1}{(L_m-1-n)!} J(n, c) \left( \frac{\gamma \gamma'}{\rho c} \right)^{n+1} \end{aligned} \quad (60)$$



and

$$\mathcal{D}^{L,L\pm 2}(\gamma, \gamma') = (2L_m + 3) \sqrt{\frac{3}{2(2L_m + 1)}} R_{\mp}; \quad (61a)$$

$$\mathcal{D}^{L,L}(\gamma, \gamma') = -\sqrt{\frac{(2L+1)(2L+3)}{(2L-1)}}. \quad (61b)$$

The alternative expression in terms of the  $\mathcal{F}$  integrals is directly obtained using the link between the  $J$  and  $\mathcal{F}$  integrals:

$$J(n, c) = \frac{(-1)^n}{\sqrt{2\pi c}} \sum_{r=0}^n (-1)^r \frac{(r+1)(r+2)}{(2r+5)!(n-r)!} \times (2c)^{r+3} \mathcal{F}_V(2r+4, c/2). \quad (62)$$

The final result is

$$\begin{aligned} & \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|) Y_2(\widehat{\tilde{w}\mathbf{x}}) || \Psi^{KL} \rangle = \delta_{L\pm 2 \text{ or } L, L'} \\ & \times \sqrt{\frac{5}{\pi}} \sqrt{\frac{L_m(L_m+1)}{\pi(2L_m+1)}} \frac{(2K+L)!(2K'+L')!}{2^{K+K'} B_{KL} B_{K'L'}} \\ & \times \left( \frac{2c\pi^N}{\det B} \right)^{3/2} \gamma^{2K+L} \gamma'^{2K'+L'} \left( -\frac{1}{c} \right)^{K+K'+L_m-1} \\ & \times \sum_{n=0}^{K+K'+L_m-1} \frac{(n+1)(n+2)}{(2n+5)!} (-2c)^n \mathcal{F}_V(2n+4, c/2) \\ & \times \sum_{l=0}^2 \sum_{k=0}^{\min(\bar{K}_l, \bar{K}'_l)} 4^k \mathcal{B}_{kl}^{L,L'} H_{n,k}^{\bar{K}_l, \bar{K}'_l, \bar{L}_l} \left( \frac{2q\gamma'}{\rho\gamma}, \frac{2q'\gamma'}{\rho\gamma'}, \frac{\rho c}{\gamma\gamma'} \right). \end{aligned} \quad (63)$$

The geometrical coefficients  $\mathcal{B}_{kl}^{L,L'}$  are independent of any parameter and looks similar to

$$\begin{aligned} \mathcal{B}_{kl}^{L,L\pm 2} &= \sqrt{\frac{3}{2}} 2^{l+\bar{l}} B_{k(L_i+l)}; \\ \mathcal{B}_{kl}^{L,L} &= -\frac{2L+1}{\sqrt{(2L-1)(2L+3)}} B_{kL} \frac{(4k+2L+2+\bar{l})}{(2k+L+1-\bar{l})}; \end{aligned} \quad (64)$$

One sees the great similarity between (63) and (40), showing once more the universality of the  $H$ -function.

The expression for the peculiar case  $K = K' = 0$  is easily derived from (60) and (62) after some algebraic manipulations

$$\begin{aligned} & \langle \Psi'^{0L'} || V(|\tilde{w}\mathbf{x}|) Y_2(\widehat{\tilde{w}\mathbf{x}}) || \Psi^{0L} \rangle = \delta_{L\pm 2 \text{ or } L, L'} \\ & \times \sqrt{\frac{5}{\pi}} \sqrt{\frac{L_m(L_m+1)}{8\pi c}} \mathcal{N}_{L_m}(L_m-1)! \mathcal{D}^{L,L'}(\gamma, \gamma') \\ & \times \sum_{n=0}^{L_m-1} \frac{(n+1)(n+2)}{(2n+5)!(L_m-1-n)!} (2c)^{n+3} \mathcal{F}_V(2n+4, c/2) \\ & \times \left( \frac{\gamma\gamma'}{\rho c} \right)^{n+1} \left( 1 - \frac{\gamma\gamma'}{\rho c} \right)^{L_m-(n+1)} \end{aligned} \quad (65)$$

with the same geometrical coefficients  $\mathcal{D}^{L,L'}$  as before (61).

The alternative derivation can be obtained using exactly the same technics that was developed for the spin-orbit potential. The explicit result looks quite sympathetic:

$$\begin{aligned} & \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|) Y_2(\widehat{\tilde{w}\mathbf{x}}) || \Psi^{KL} \rangle = \delta_{L\pm 2 \text{ or } L, L'} \sqrt{\frac{5}{\pi}} \gamma\gamma' \\ & \times \frac{(2K+L)!(2K'+L')!}{B_{KL} B_{K'L'}} \left( \frac{\alpha\pi^N}{\det B} \right)^{3/2} \sqrt{\frac{L_m(L_m+1)}{2L_m+1}} \\ & \times \sum_{n=0}^{K+K'+L_m-1} \left( \frac{\alpha}{2c} \right)^{n+1} J(n, \alpha, c) \sum_{l=0}^2 \sum_{k=0}^{\min(\bar{K}_l, \bar{K}'_l)} \\ & \times \frac{2^{2k+\bar{L}_l}}{(2k+\bar{L}_l)!} \mathcal{A}_{kl}^{L,L'}(\gamma, \gamma') F_{n,k}^{\bar{K}_l, \bar{K}'_l, \bar{L}_l}(\bar{q}, \bar{q}', \gamma, \gamma') \end{aligned} \quad (66)$$

where the dynamical integral  $J(n, \alpha, c)$  is given by (12) with the same value of the  $Q_n(x)$  as before (55). The coefficients  $\mathcal{A}_{kl}^{L,L'}$  are still given by (56) and the indices  $\bar{K}_l, \bar{K}'_l, \bar{L}_l$  by (57). The  $F$ -function (15) appears naturally in this expression.

The special case  $K = K' = 0$  is particularly simple since it does not need any summation

$$\begin{aligned} & \langle \Psi'^{0L'} || V(|\tilde{w}\mathbf{x}|) Y_2(\widehat{\tilde{w}\mathbf{x}}) || \Psi^{0L} \rangle = \delta_{L\pm 2 \text{ or } L, L'} \\ & \times \sqrt{\frac{5}{4\pi}} \sqrt{L_m(L_m+1)} \mathcal{N}_{L_m}(L_m-1)! \\ & \times \mathcal{D}^{L,L'}(\gamma, \gamma') \alpha^{3/2} \left( \frac{\alpha}{1-\alpha} \right)^{L_m} J(L_m-1, \alpha, c) \end{aligned} \quad (67)$$

with the same geometrical coefficients  $\mathcal{D}^{L,L'}$  as before (61).

The last thing that remains to do is to express the reduced matrix elements in terms of the  $\mathcal{F}$  integrals. This is easily done using the expansion

$$\begin{aligned} J(n, \alpha, c) &= (-1)^n \sqrt{\frac{\alpha}{2\pi c}} \sum_{r=0}^n \mathcal{F}_V(2r+4, c/2) \\ & \times (-1)^r \frac{(r+1)(r+2)}{(2r+5)!(n-r)!} \left( \frac{2c}{\alpha} \right)^{r+3}. \end{aligned} \quad (68)$$

One gets

$$\begin{aligned} & \langle \Psi'^{K'L'} || V(|\tilde{w}\mathbf{x}|) Y_2(\widehat{\tilde{w}\mathbf{x}}) || \Psi^{KL} \rangle = \delta_{L\pm 2 \text{ or } L, L'} \sqrt{\frac{5}{\pi}} \\ & \times \sqrt{\frac{L_m(L_m+1)}{\pi(2L_m+1)}} \frac{(2K+L)!(2K'+L')!}{B_{KL} B_{K'L'}} \left( \frac{2c\pi^N}{\det B} \right)^{3/2} \gamma\gamma' \\ & \times \sum_{n=0}^{K+K'+L_m-1} \frac{(n+1)(n+2)}{(2n+5)!} \mathcal{F}_V(2n+4, c/2) \sum_{l=0}^2 \sum_{k=0}^{\min(\bar{K}_l, \bar{K}'_l)} \\ & \times \frac{2^{2k+\bar{L}_l}}{(2k+\bar{L}_l)!} \mathcal{A}_{kl}^{L,L'}(\gamma, \gamma') P_{n,k}^{\bar{K}_l, \bar{K}'_l, \bar{L}_l} \left( \bar{q}, \bar{q}', \gamma, \gamma', \frac{-\alpha\gamma'^2}{2cq'} \right) \end{aligned} \quad (69)$$

where, again, the  $P$  function (18) enters the game.

Starting with (67), using (68) and rearranging the summations allows to obtain the matrix element for the special case  $K = K' = 0$  under the form already proposed (65). This is a fantastic check of the calculation.

## V. CONCLUSIONS

In this paper, we pursued the work begun in SV and SBM and proposed general expressions for the matrix elements of spin dependent operators on correlated gaussian wave functions with natural parity. This type of basis wave functions are the basic ingredients of the stochastic variational method which allows to get very precise results for few-body systems.

The corresponding formulae are able to treat the matrix elements of the Hamiltonian for a system with an arbitrary number of particles and for states with arbitrary angular momentum in a closed form. This is very important from the numerical point of view; the only purely numerical work is the computation of a one dimensional integral containing the form of the potential. Moreover, for most of the usual potentials, the corresponding integrals are themselves analytical, so that all the matrix elements are obtained in a closed form. The solution for the Schrödinger equation is subsequently obtained as a generalized eigenvalue problem which is very well under control numerically.

The only spin dependent potentials that are treated in this paper are the spin-orbit – symmetric and antisymmetric– and tensor forces. They are, by far, the most common for atomic, nuclear and hadronic spectroscopy. The spin matrix elements are computed with standard Racah algebra and we focus here on space reduced matrix elements.

We proposed two ways to calculate the matrix elements : one approach based on the underlying philosophy of SV where the symmetry properties are obvious, and another approach developed in SBM where the symmetry properties are less transparent but more efficient numerically. Since the link between both is far from obvious, a comparison between both formulations is indeed a very good check of the numerical codes. We gave the formulae for the general correlated Gaussians  $K \neq 0$  but also for the special case  $K = 0$  for which they are much simpler. In this case, all the matrix elements have the remarkable feature to be proportional to the overlap matrix element.

In each approach, we also proposed two expressions

- one based on a numerical integral of type  $J$  which lead to the simplest formulation but which has the drawback to be given in terms of combinations of Hermite polynomials;
- one based on a numerical integral of type  $\mathcal{F}$  which gives a slightly more complicated formulation but with an easy and universal type of integral.

In the special case  $K = 0$ , both formulations are of the same difficulty so that the second approach is much more convenient.

Again, all these alternative expressions for the computation of the matrix elements allow very good checks of the results.

The very sympathetic feature of the method proposed in this paper is that it relies on universal geometrical functions that can be built once and for all and that can be employed whatever the potential under consideration. Moreover the arguments that enter these functions depend on the free parameters of the basis wave function and the particular pair of particles under consideration only and are independent of the form of the potential for a given pair. Consequently all types or combinations of potentials can be treated on the same footing in a single type of summation. This is very important to shorten the computer time needed for the evaluation of the matrix elements.

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## APPENDIX A: SOME MATRIX ELEMENTS FOR GENERATING FUNCTIONS

In order to calculate matrix elements of some operator in the basis of correlated Gaussians, the first step is to calculate the matrix elements of this operator on the generating functions. Expressing the coordinates of the particles in terms of the Jacobi coordinates  $\mathbf{x}$ , the most general form for the spatial part of the operator is  $V(\tilde{w}\mathbf{x})$ . Thus, it is natural to compute the matrix element of the operator  $\delta(\tilde{w}\mathbf{x} - \mathbf{r})$ . Such an expression can be found in SV.

However, it appears that, in any case, the form of the operator is rather  $V(|\tilde{w}\mathbf{x}|) \times F(\tilde{w}\mathbf{x})$  where the function  $F(\tilde{w}\mathbf{x})$  is very specific and given once for all. The element can be calculated from the expression in term of three dimensional Dirac function, but this needs evaluating a three dimensional integral. We find more convenient to calculate the matrix elements on generating functions for an operator of type  $\delta(|\tilde{w}\mathbf{x}| - r) \times F(\tilde{w}\mathbf{x})$ . The angular integration is reported entirely on the specific function  $F$  and the remaining job is just a one dimensional radial integral. The resulting expressions are not given in SV, and we think that they can be interesting for the reader.

## 1. Case of spherical harmonics

A common case concerns spherical harmonics  $F(\tilde{w}\mathbf{x}) = Y_{\lambda\mu}(\tilde{w}\mathbf{x})$ . The central potential corresponds to the case  $\lambda = 0$ , while the tensor case corresponds to  $\lambda = 2$ .

The technics to calculate the matrix element is based on a well-known trick. The generating functions are expressed in terms of Gaussians and grouped into a single Gaussian of the form  $\exp(-\tilde{\mathbf{x}} \cdot B\mathbf{x} + \tilde{\mathbf{v}} \cdot \mathbf{x})$ , where  $B = A + A'$  and  $\mathbf{v} = \mathbf{s} + \mathbf{s}'$ . The  $B$  matrix, which is symmetric and definite positive, is diagonalized to a matrix  $D$  with help of an orthogonal matrix  $T$ . Instead of  $\mathbf{x}$  variables, we use new variables  $\mathbf{z}$ , defined by  $\mathbf{z} = D^{1/2}T\mathbf{x}$ . The exponential takes the form  $\exp(-\tilde{\mathbf{z}} \cdot \mathbf{z} + \tilde{\mathbf{u}} \cdot \mathbf{z})$  and the argument of the Dirac function becomes  $|\tilde{a}\mathbf{z}| - r$ . We then change again variables to  $\mathbf{Z} = U\mathbf{z}$ , where  $U$  is an orthogonal matrix so that  $\tilde{\mathbf{z}} \cdot \mathbf{z} = \tilde{\mathbf{Z}} \cdot \mathbf{Z}$ . One can use the freedom left to the form of  $U$  to choose a peculiar form such as  $\mathbf{Z}_1$  is proportional to  $\tilde{a}\mathbf{z}$  (the interested reader can refer to BSM for the notations). The rest of the derivation is standard and straightforward. To perform the angular integration for the spherical harmonic, it is convenient to expand the corresponding  $\exp(\mathbf{V}_1 \cdot \mathbf{Z}_1)$  term as the usual plane wave development in terms of spherical harmonics; this one introduces the spherical modified Bessel function  $i_l(z) = \sqrt{\pi/(2z)} I_{l+1/2}(z)$ .

The final result is

$$\left\langle g(\mathbf{s}', A'; \mathbf{x}) | \delta(|\tilde{w}\mathbf{x}| - r) Y_{\lambda\mu}(\tilde{w}\mathbf{x}) | g(\mathbf{s}, A; \mathbf{x}) \right\rangle = \frac{4}{\sqrt{\pi}} \frac{\mathcal{M}_0}{(\tilde{w}B^{-1}w)^{3/2}} r^2 \mathcal{I}_\lambda(w, B, \mathbf{v}) Y_{\lambda\mu}(\tilde{w}B^{-1}\mathbf{v}), \quad (\text{A1})$$

in which

$$\mathcal{M}_0 = \left( \frac{\pi^N}{\det B} \right)^{3/2} \exp\left( \frac{1}{4} \mathbf{v} \cdot \tilde{B}^{-1} \mathbf{v} \right) \quad (\text{A2})$$

is the matrix element corresponding to the overlap of generating functions with

$$B = A + A' \quad ; \quad \mathbf{v} = \mathbf{s} + \mathbf{s}' \quad (\text{A3})$$

and

$$\mathcal{I}_\lambda(w, B, \mathbf{v}) = i_\lambda \left( \frac{r|\tilde{w}B^{-1}\mathbf{v}|}{\tilde{w}B^{-1}w} \right) \exp\left( -\frac{r^2 + \frac{1}{4}(\tilde{w}B^{-1}\mathbf{v})^2}{\tilde{w}B^{-1}w} \right). \quad (\text{A4})$$

## 2. Angular momentum

In the case of angular momentum, the  $F$  function is a bit more complicated since it contains, in addition to the Jacobi variables, the derivatives of them. Explicitly, it is the vector product  $F = \tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}$ . The momentum  $\boldsymbol{\pi} = -i\partial/\partial\mathbf{x}$  needs to calculate the derivative of the generating ket function. Fortunately this derivative is still proportional to a Gaussian, so that the same procedure

as before can be adopted. There are additional terms which can be treated exactly. The vector product being a tensor of order 1, it is expected that the  $i_1$  function appears; this is indeed the case.

Explicitly, one finds

$$\left\langle g(\mathbf{s}', A'; \mathbf{x}) | \delta(|\tilde{w}\mathbf{x}| - r) (\tilde{w}\mathbf{x} \times \tilde{\zeta}\boldsymbol{\pi}) | g(\mathbf{s}, A; \mathbf{x}) \right\rangle = -i \frac{4}{\sqrt{\pi}} \times \frac{\mathcal{M}_0 r^3}{(\tilde{w}B^{-1}w)^{3/2} |\tilde{w}B^{-1}\mathbf{v}|} \mathcal{I}_1(w, B, \mathbf{v}) [(\tilde{w}B^{-1}\mathbf{v}) \times (\tilde{\zeta}\mathbf{y})], \quad (\text{A5})$$

where, in addition to the quantities previously defined, we have a new variable

$$\mathbf{y} = A'B^{-1}\mathbf{s} - AB^{-1}\mathbf{s}'. \quad (\text{A6})$$

One sees that in both cases, we have more or less the same numerical quantities to compute, and this is a very important feature in the efficiency of the numerical codes.

## APPENDIX B: A SPECIAL SERIES EXPANSION

During the calculation of the interesting matrix elements, it is very helpful to have a series expansion for the function  $\exp(-az^2)i_l(bz)$ . The case  $l = 0$  corresponds to a central potential, while  $l = 1$  appears for a spin-orbit potential. The expression for  $l = 0$  is given in SV (formula (A.125)) while expression for  $l = 1$  is also in SV (formula (A.164)).

However, for the tensor operator, we need the expression for  $l = 2$ . This expression is missing in SV. Moreover the expressions proposed in SV are under a form that is not transparent for generalization. To fill this gap, we propose here an interesting formula, valid for any  $l$ . It is expressed in terms of Hermite polynomials of odd order  $H_{2n+1}$ . These polynomials occur naturally since they come as by-product of their generating function. More precisely

$$e^{-s^2+2sx} = \sum_{n=0}^{\infty} H_n(x) \frac{s^n}{n!}. \quad (\text{B1})$$

The first thing to do is to use a new variable  $u = 2\sqrt{a}z$ , so that  $\exp(-az^2)i_l(bz) = \exp(-u^2/4)i_l(\alpha u)$  is now function of only one parameter  $\alpha = b/(2\sqrt{a})$ . The series expansion of  $i_l(x)$  is a sum of a polynomial in  $x$  times a term like  $e^x$  and another polynomial in  $x$  times a term like  $e^{-x}$ , both divided by some power of  $x$  (see ref. [7]). For small values of  $l$  these polynomials are not complicated and formula (B1) can be applied safely. One can recast the searched expression under the form:

$$\exp(-u^2/4)i_l(\alpha u) = \frac{1}{2\alpha^{l+1}} \sum_{p=0}^{\infty} (u/2)^{2p+l} K_p^{(l)}(\alpha). \quad (\text{B2})$$

As it comes, the  $K_p^{(l)}(\alpha)$  is expressed in terms of Hermite polynomials multiplied by finite powers of  $\alpha$ . It is tricky to remove this dependence using the recursion formula on Hermite polynomials:

$$2xH_n(x) = H_{n+1}(x) + 2nH_{n-1}(x). \quad (\text{B3})$$

For small values of  $l$ , it appears that the  $K_p^{(l)}$  can be put under the form:

$$K_p^{(l)}(x) = \frac{l!}{p!} \sum_{r=0}^l \frac{(p+r)!}{r!(l-r)!} \frac{H_{2p+2r+1}(x)}{(2p+2r+1)!}. \quad (\text{B4})$$

What remains to do is to prove the general formula valid for any  $l$ . This can be done by induction, using the well known recursion relation

$$i_{l+1}(z) = i_{l-1}(z) - \frac{2l+1}{z} i_l(z). \quad (\text{B5})$$

To get the final result we come back to the variable  $z$  instead of  $u$ . Thus, the series expansion of important use is given by

$$e^{-az^2} i_l(bz) = \frac{1}{2\alpha^{l+1}} \sum_{p=0}^{\infty} (\sqrt{a}z)^{2p+l} K_p^{(l)}(\alpha); \quad \alpha = \frac{b}{2\sqrt{a}} \quad (\text{B6})$$

with the  $K_p^{(l)}$  function defined by (B4).

Of some interest is also the series expansion of Hermite polynomials appearing in the  $K_p^{(l)}(x)$  functions; explicitly

$$\frac{H_{2n+1}(x)}{(2n+1)!} = \sum_{r=0}^n (-1)^{n+r} \frac{(2x)^{2r+1}}{(2r+1)!(n-r)!}. \quad (\text{B7})$$

### APPENDIX C: INTEGRAL OVER ANGULAR VARIABLES

In the process of calculation of the matrix elements in terms of those concerned by the generating functions, we are faced to calculate the following integral

$$\mathcal{I}_{\lambda\mu}^{L'M',LM,n}(a',a) = \int d\hat{e} d\hat{e}' Y_{L'M'}^*(\hat{e}') Y_{LM}(\hat{e}) \mathcal{Y}_{\lambda\mu}(a\mathbf{e} + a'\mathbf{e}') (\mathbf{e} \cdot \mathbf{e}')^n \quad (\text{C1})$$

where  $\mathbf{e}$  and  $\mathbf{e}'$  are unit vectors ( $|\mathbf{e}| = 1 = |\mathbf{e}'|$ ) and  $\mathcal{Y}_{\lambda\mu}(\mathbf{r}) = r^\lambda Y_{\lambda\mu}(\hat{\mathbf{r}})$  is a solid harmonic. The integration is done on angular coordinates of  $\mathbf{e}$  and  $\mathbf{e}'$ .

Because of rotational properties, we guess that this integral is proportional to a Clebsch-Gordan coefficient. Thus, let us define a reduced matrix element  $\mathcal{I}_{\lambda}^{L',L,n}(a',a)$  through the usual form ( $\hat{L} = \sqrt{2L+1}$ )

$$\mathcal{I}_{\lambda\mu}^{L'M',LM,n}(a',a) = \frac{\langle LM\lambda\mu | L'M' \rangle}{\hat{L}'} \mathcal{I}_{\lambda}^{L',L,n}(a',a). \quad (\text{C2})$$

The evaluation of this quantity is based on three fundamental formulae

1.

$$\mathcal{Y}_{\lambda\mu}(a\mathbf{e} + a'\mathbf{e}') = \sum_{l=0}^{\lambda} Z_l^{\lambda} a^l a'^{\lambda-l} [Y_l(\hat{e}) Y_{\lambda-l}(\hat{e}')]_{\lambda\mu}, \quad (\text{C3})$$

where the geometrical coefficient  $Z_l^{\lambda}$  takes the value

$$Z_l^{\lambda} = \sqrt{\frac{4\pi(2\lambda+1)!}{(2l+1)!(2\lambda-2l+1)!}}. \quad (\text{C4})$$

Note that in obtaining (C3), we used the fact that  $\mathbf{e}$  and  $\mathbf{e}'$  are unit vectors. Note also the symmetry of the  $Z$  coefficient:  $Z_l^{\lambda} = Z_{\lambda-l}^{\lambda}$ .

2.

$$(\mathbf{e} \cdot \mathbf{e}')^n = \sum_{k,p \geq 0, 2k+p=n} B_{kp} (-1)^p \sqrt{2p+1} [Y_p(\hat{e}) Y_p(\hat{e}')]_{00} \quad (\text{C5})$$

which is valid for unit vectors  $\mathbf{e}$  and  $\mathbf{e}'$ . The geometrical coefficient  $B_{kp}$  is defined through (8). One must always have  $k$  integer  $\geq 0$  and the index  $p$  must have the same parity than  $n$  in (C5).

3.

$$[Y_{l_1}(\hat{e}) Y_{l_2}(\hat{e})]_{lm} = \frac{\hat{l}_1 \hat{l}_2}{\sqrt{4\pi} \hat{l}} \langle l_1 0 l_2 0 | l 0 \rangle Y_{lm}(\hat{e}). \quad (\text{C6})$$

Inserting those relations in the searched integral leads, after some manipulations, to the final result:

$$\begin{aligned} \mathcal{I}_{\lambda}^{L',L,n}(a',a) &= \frac{\hat{\lambda}}{4\pi} \sum_{l=0}^{\lambda} (-1)^l \widehat{l\lambda-l} Z_l^{\lambda} a^l a'^{\lambda-l} \\ &\times \sum_{\substack{k,p \geq 0 \\ 2k+p=n}} B_{kp} (2p+1) \langle l 0 p 0 | L 0 \rangle \\ &\times \langle \lambda - l 0 p 0 | L' 0 \rangle \begin{Bmatrix} \lambda - l & l & \lambda \\ L & L' & p \end{Bmatrix} \end{aligned} \quad (\text{C7})$$

including usual Clebsch-Gordan and 6J coefficients.

For the tensor operator, we need this integral with the peculiar value  $\lambda = 2$ . Using the symmetry properties of Clebsch-Gordan coefficients, it is easy to check that  $L$  and  $L'$  must have the same parity, and, because of the angular momentum coupling, this means that  $L' = L \pm 2$  or  $L' = L$ . Inserting in (C7) the special values for the Clebsch-Gordan and 6J coefficients, one gets the value of the integral in this case

$$\begin{aligned} \mathcal{I}_2^{L \pm 2, L, n}(a',a) &= \sqrt{\frac{15L_m(L_m+1)}{8\pi(2L_m+1)}} \\ &\times \sum_{l=0}^2 \sum_{k \geq 0} 2^l B_{k(L_i+l)} a_{\pm}^l a'_{\pm}^{2-l} \delta_{2k+L_i, n-l}, \end{aligned} \quad (\text{C8a})$$

$$\mathcal{I}_2^{L,L,n}(a', a) = -\sqrt{\frac{5L(L+1)(2L+1)}{4\pi(2L-1)(2L+3)}} \times \sum_{l=0}^2 \sum_{k \geq 0} \frac{4k+2L+2+\bar{l}}{2^{1-\bar{l}}(2k+L+1-\bar{l})} B_{kL} a^l a'^{2-l} \delta_{2k+L,n+\bar{l}}, \quad (\text{C8b})$$

with  $L_m, L_i, \bar{l}$  defined in (58) and the quantities

$$(a_+, a'_+) = (a, a'); \quad (a_-, a'_-) = (a', a). \quad (\text{C9})$$

For the  $LS$  operator, we need such an integral with  $i(\mathbf{e} \times \mathbf{e}')_\mu$  instead of  $\mathcal{Y}_{\lambda\mu}(a\mathbf{e} + a'\mathbf{e}')$ . Since  $i(\mathbf{e} \times \mathbf{e}')_\mu = \frac{4\pi\sqrt{2}}{3}[\mathcal{Y}_1(\mathbf{e})\mathcal{Y}_1(\mathbf{e}')]_{1\mu}$ , most of the calculations needed before can be applied as well. One finds

$$\int d\hat{e} d\hat{e}' Y_{L'M'}^*(\hat{e}') Y_{LM}(\hat{e}) [i(\mathbf{e} \times \mathbf{e}')_\mu] (\mathbf{e} \cdot \mathbf{e}')^n = \delta_{LL'} \frac{\sqrt{L(L+1)}}{n+1} \langle L M 1 \mu | L' M' \rangle \sum_{k \geq 0} B_{kL} \delta_{2k+L,n+1}. \quad (\text{C10})$$

#### APPENDIX D: SPIN REDUCED ELEMENTS FOR 3-BODY SYSTEMS

In this section we present the spin reduced matrix elements for the 3-body problem that appear for the most important spin dependent operators. In some papers we can find them but most of the time they are given for spin 1/2 particles (nucleons or quarks). Here we have in mind the general 3-body problem (in particular one can consider hybrid states including gluons with spin 1, or pions with spin 0). The spin for the particle  $i$  is denoted  $\mathbf{s}_i$ .

The spin function for the the 3-body problem is chosen as

$$|\chi_S(1, 2, 3)\rangle = |[(s_1 s_2)_{S_{12}} s_3]_S\rangle \quad (\text{D1})$$

where  $S_{12}$  is the partial coupling of the  $(1-2)$  pair.

We want to calculate the reduced matrix elements  $\langle \chi_{S'} | \hat{O} | \chi_S \rangle$  for the interesting spin operators  $\hat{O}$ . In practice, we will consider

- one-body spin operators of the form  $\hat{O}_i(1, 2, 3) = \hat{O}_i(i) \otimes \hat{1}(j) \otimes \hat{1}(k)$ , where  $\hat{1}(j)$  is the unit operator for particle  $j$  and where  $\hat{O}_i(i)$  concerns the particle  $i$  only and has a given tensorial character.
- two-body spin operators of the form  $\hat{O}_{ij}(1, 2, 3) = \hat{O}_{ij}(i, j) \otimes \hat{1}(k)$ . The operator  $\hat{O}_{ij}(i, j)$  concerns the pair  $(ij)$  and results itself from the coupling  $[\hat{O}_i(i) \otimes \hat{O}_j(j)]$ .

To obtain the searched matrix elements is just a matter of Racah recoupling. Very few formulae are indeed necessary. The most important one concerns the case when

the operator is the tensor product of two operators acting on two distinct subsystems. Explicitly ( $\hat{J} = \sqrt{2J+1}$ )

$$\langle (j'_1 j'_2)_{J'} | [O_1^{k_1} \otimes O_2^{k_2}]_k | (j_1 j_2)_J \rangle = \hat{j}' \hat{j} \hat{k} \begin{Bmatrix} j_1 & j_2 & J \\ k_1 & k_2 & k \\ j'_1 & j'_2 & J' \end{Bmatrix} \langle j'_1 | O_1^{k_1} | j_1 \rangle \langle j'_2 | O_2^{k_2} | j_2 \rangle. \quad (\text{D2})$$

Very often, we are in the special case where  $O_2^{k_2} = \hat{1}(2)$ ; then one uses the special value

$$\langle j' | \hat{1} | j \rangle = \hat{j} \delta_{j'j} \quad (\text{D3})$$

to get a simplified relation

$$\langle (j'_1 j'_2)_{J'} | O_1^{k_1} | (j_1 j_2)_J \rangle = \delta_{j'_2 j_2} \langle j'_1 | O_1^{k_1} | j_1 \rangle \times (-1)^{j'_1 + j'_2 + J + k_1} \hat{j}' \hat{j} \begin{Bmatrix} j'_1 & k_1 & j_1 \\ J & j_2 & J' \end{Bmatrix}. \quad (\text{D4})$$

Of some utility is also the following formula

$$\langle j' | \hat{J} | j \rangle = \hat{j} \sqrt{j(j+1)} \delta_{j'j}. \quad (\text{D5})$$

With these tools, the calculation of the various reduced matrix elements is just a matter of algebraic calculus.

When we consider the spin-orbit correction of a confining QCD potential, the spin operators that intervene are simply the one-body  $\mathbf{s}_i$  operators. Application of the above formulae leads to

$$\langle \chi_{S'} | \mathbf{s}_1 | \chi_S \rangle = (-1)^{s_1 + s_2 + s_3 + S_{12} + S'_{12} + S} \sqrt{s_1(s_1+1)} \times \widehat{s_1} \widehat{S_{12}} \widehat{S'_{12}} \widehat{S} \widehat{S'} \begin{Bmatrix} S'_{12} & 1 & S_{12} \\ S & s_3 & S' \end{Bmatrix} \begin{Bmatrix} s_1 & 1 & s_1 \\ S_{12} & s_2 & S'_{12} \end{Bmatrix} \quad (\text{D6})$$

$$\langle \chi_{S'} | \mathbf{s}_2 | \chi_S \rangle = (-1)^{s_1 + s_2 - s_3 - S} \sqrt{s_2(s_2+1)} \times \widehat{s_2} \widehat{S_{12}} \widehat{S'_{12}} \widehat{S} \widehat{S'} \begin{Bmatrix} S'_{12} & 1 & S_{12} \\ S & s_3 & S' \end{Bmatrix} \begin{Bmatrix} s_2 & 1 & s_2 \\ S_{12} & s_1 & S'_{12} \end{Bmatrix} \quad (\text{D7})$$

$$\langle \chi_{S'} | \mathbf{s}_3 | \chi_S \rangle = (-1)^{S' + S_{12} + s_3 + 1} \delta_{S'_{12}, S_{12}} \times \sqrt{s_3(s_3+1)} \widehat{s_3} \widehat{S} \widehat{S'} \begin{Bmatrix} s_3 & 1 & s_3 \\ S & S_{12} & S' \end{Bmatrix}. \quad (\text{D8})$$

For the two-body symmetric spin-orbit potential, the spin operator is simply  $\mathbf{S}_{ij} = \mathbf{s}_i + \mathbf{s}_j$ . The reduced matrix elements for this operator are easily obtained by addition of the corresponding  $\mathbf{s}_i$  and  $\mathbf{s}_j$  elements as given previously.

For the two-body antisymmetric spin-orbit potential, the spin operator is simply  $\mathbf{\Delta}_{ij} = \mathbf{s}_i - \mathbf{s}_j$ . The reduced matrix elements for this operator are easily obtained by difference of the corresponding  $\mathbf{s}_i$  and  $\mathbf{s}_j$  elements as given previously.

Lastly for the two-body tensor operator the spin operator is  $\mathbf{S}_{ij}$  with two possible expressions for the operator (see Eq. (51)). After long but straightforward calculations, one gets

for  $\mathcal{S}_{ij} = (\mathbf{s}_i \otimes \mathbf{s}_j)_2$

$$\begin{aligned} \langle \chi'_{S'} | (\mathbf{s}_1 \otimes \mathbf{s}_2)_2 | \chi_S \rangle &= \widehat{s}_1 \widehat{s}_2 \sqrt{5s_1 s_2 (s_1 + 1)(s_2 + 1)} \\ &\times (-1)^{S+S'_{12}+s_3+1} \widehat{S'_{12}} \widehat{S'_{12}} \widehat{S} \widehat{S'} \\ &\times \begin{Bmatrix} S'_{12} & 2 & S_{12} \\ S & s_3 & S' \end{Bmatrix} \begin{Bmatrix} s_1 & s_2 & S_{12} \\ 1 & 1 & 2 \\ s_1 & s_2 & S'_{12} \end{Bmatrix}, \end{aligned} \quad (\text{D9})$$

$$\begin{aligned} \langle \chi'_{S'} | (\mathbf{s}_2 \otimes \mathbf{s}_3)_2 | \chi_S \rangle &= \sqrt{5s_2 s_3 (s_2 + 1)(s_3 + 1)} \\ &\times \widehat{s}_2 \widehat{s}_3 \widehat{S'_{12}} \widehat{S'_{12}} \widehat{S} \widehat{S'} \sum_{k,k'} (-1)^{S+k+s_1+1} \\ &\times (2k+1)(2k'+1) \begin{Bmatrix} s_1 & s_2 & S'_{12} \\ s_3 & S' & k' \end{Bmatrix} \begin{Bmatrix} s_1 & s_2 & S_{12} \\ s_3 & S & k \end{Bmatrix} \\ &\times \begin{Bmatrix} k' & 2 & k \\ S & s_1 & S' \end{Bmatrix} \begin{Bmatrix} s_2 & s_3 & k \\ 1 & 1 & 2 \\ s_2 & s_3 & k' \end{Bmatrix}. \end{aligned} \quad (\text{D10})$$

for  $\mathcal{S}_{ij} = (\mathbf{S}_{ij} \otimes \mathbf{S}_{ij})_2$

$$\begin{aligned} \langle \chi'_{S'} | (\mathbf{S}_{12} \otimes \mathbf{S}_{12})_2 | \chi_S \rangle &= \delta_{S_{12}, S'_{12}} \sqrt{5} S_{12} (S_{12} + 1) (2S_{12} + 1) \\ &\times (-1)^{S+s_3+1-S_{12}} \widehat{S} \widehat{S'} \\ &\times \begin{Bmatrix} S_{12} & 2 & S_{12} \\ S & s_3 & S' \end{Bmatrix} \begin{Bmatrix} 1 & 1 & 2 \\ S_{12} & S_{12} & S_{12} \end{Bmatrix}, \end{aligned} \quad (\text{D11})$$

$$\begin{aligned} \langle \chi'_{S'} | (\mathbf{S}_{23} \otimes \mathbf{S}_{23})_2 | \chi_S \rangle &= \sqrt{5} \widehat{S'_{12}} \widehat{S'_{12}} \widehat{S} \widehat{S'} \\ &\times \sum_k (-1)^{S-k+s_3+1} k(k+1)(2k+1)^2 \\ &\times \begin{Bmatrix} 1 & 1 & 2 \\ k & k & k \end{Bmatrix} \begin{Bmatrix} k & 2 & k \\ S & s_3 & S' \end{Bmatrix} \\ &\times \begin{Bmatrix} s_1 & s_2 & S_{12} \\ s_3 & S & k \end{Bmatrix} \begin{Bmatrix} s_1 & s_2 & S'_{12} \\ s_3 & S' & k \end{Bmatrix}. \end{aligned} \quad (\text{D12})$$

The matrix element  $\langle \chi'_{S'} | \mathcal{S}_{13} | \chi_S \rangle$  is obtained from the element  $\langle \chi'_{S'} | \mathcal{S}_{23} | \chi_S \rangle$  with the interchange  $1 \leftrightarrow 2$  and adding a phase  $(-1)^{S_{12}-S'_{12}}$ .

## APPENDIX E: SUMMARY OF PREVIOUS KNOWN FORMULAE

This section is devoted to the presentation of formulae that are not new since they have been derived previously either in SV or in SBM. Nevertheless we find convenient to give a brief summary of them for two main reasons:

- to achieve some unity in the paper since with the bulk of formulae given in this section and in the rest of this work, the reader has all the necessary tools for solving the few-problem with the most common types of potentials.

- we want to show that whatever the dynamical quantities that are considered, they all rely on the same geometrical coefficients and a few of universal geometrical functions.

All the dynamical parameters that appear in this section have been defined previously in the paper.

### 1. Overlap

The overlap between basis states  $\mathcal{N}_{K'KL} = \langle \psi_{K'LM}(u', A') | \psi_{KLM}(u, A) \rangle$  is a crucial ingredient in the equation of motion. Since the basis states are non orthogonal, there is no reason that such an element is diagonal.

As shown in SV, the overlap is [SV, (A.6) page 248]

$$\begin{aligned} \mathcal{N}_{K'KL} &= \frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}} \left( \frac{\pi^N}{\det B} \right)^{3/2} \\ &\times \sum_{k=0}^{\min(K,K')} B_{kL} \frac{q^{K-k}}{(K-k)!} \frac{q'^{K'-k}}{(K'-k)!} \frac{\rho^{2k+L}}{(2k+L)!} \end{aligned} \quad (\text{E1})$$

For the important peculiar case  $K' = K = 0$ , this formula simplifies a lot and we are left with [SV (A.7) page 249]:

$$\mathcal{N}_{00L} = \mathcal{N}_L = \frac{(2L+1)!!}{4\pi} \left( \frac{\pi^N}{\det B} \right)^{3/2} \rho^L. \quad (\text{E2})$$

### 2. Non relativistic kinetic energy

The intrinsic kinetic energy operator  $T_{NR}$  can be cast under the form

$$T_{NR} = \frac{1}{2} \sum_{i,j=1}^N \Lambda_{ij} \pi_i \cdot \pi_j = \frac{1}{2} \tilde{\pi} \cdot \Lambda \pi \quad (\text{E3})$$

The final result for this operator is [see SV, (A.10) page 250]

$$\begin{aligned} \langle \psi_{K'LM}(u', A') | \tilde{\pi} \cdot \Lambda \pi | \psi_{KLM}(u, A) \rangle &= \\ &\times \frac{(2K'+L)!(2K+L)!}{B_{K'L}B_{KL}} \left( \frac{\pi^N}{\det B} \right)^{3/2} \sum_{k=0}^{\min(K,K')} B_{kL} \\ &\times [Rqq'\rho + P(K-k)q'\rho + P'(K'-k)q\rho + Q(2k+L)qq'] \\ &\times \frac{q^{K-k-1}}{(K-k)!} \frac{q'^{K'-k-1}}{(K'-k)!} \frac{\rho^{2k+L-1}}{(2k+L)!} \end{aligned} \quad (\text{E4})$$

with the numbers  $P, P', Q, R$  defined by

$$\begin{aligned} P &= -\tilde{u}B^{-1}A'\Lambda A'B^{-1}u ; & P' &= -\tilde{u}'B^{-1}A\Lambda AB^{-1}u'; \\ Q &= 2\tilde{u}'B^{-1}A\Lambda A'B^{-1}u ; & R &= 6\text{Tr}(AB^{-1}A'\Lambda). \end{aligned} \quad (\text{E5})$$

Again, the formula for the special case  $K = K' = 0$  is much simpler

$$\langle \psi_{0LM}(u', A') | \tilde{\pi} \cdot \Lambda \pi | \psi_{0LM}(u, A) \rangle = \mathcal{N}_L \left( R + L \frac{Q}{\rho} \right). \quad (\text{E6})$$

In SBM, we gave also the matrix elements for a semi-relativistic kinetic energy operator but, since it is not of use in atomic and nuclear physics we do not report it here. The interested reader will find it under the formula (44) of SBM.

### 3. Central potentials

In the most interesting cases, the potentials appearing in the few-body problem are either one-body potentials or two-body potentials. With the same arguments than those developed in the second section, the most general form of the central potential is a sum of terms like  $V(|\tilde{w}\mathbf{x}|)$ .

The expression given in SV looks similar to [SV, (A.128) page 282]:

$$\begin{aligned} \langle \psi_{K'LM}(u', A') | V(|\tilde{w}\mathbf{x}|) | \psi_{KLM}(u, A) \rangle = \\ \left( \frac{\pi^N}{\det B} \right)^{3/2} \frac{(2K' + L)! (2K + L)!}{B_{K'L} B_{KL}} \sum_{n=0}^{K+K'+L} \frac{J(n, c)}{c^n} \\ \times \sum_{k=0}^{\min(K, K')} B_{kL} F_{K-k, K'-k, 2k+L}^n(q, q', \rho, \gamma, \gamma') \end{aligned} \quad (\text{E7})$$

which, for the peculiar case  $K = K' = 0$  reduces to [SV, (A.130) page 282]

$$\langle \psi_{0LM} | V(|\tilde{w}\mathbf{x}|) | \psi_{0LM} \rangle = \mathcal{N}_L L! \sum_{n=0}^L \frac{J(n, c)}{(L-n)!} \left( \frac{\gamma\gamma'}{\rho c} \right)^n. \quad (\text{E8})$$

Expressed in terms of the  $\mathcal{F}$  integrals, the value can be found in SBM [SBM, (C14) page 10]

$$\begin{aligned} \langle \psi_{K'LM}(u', A') | V(|\tilde{w}\mathbf{x}|) | \psi_{KLM}(u, A) \rangle = \\ \frac{(2K' + L)! (2K + L)!}{\sqrt{2\pi} 2^{K+K'-1} B_{K'L} B_{KL}} \left( \frac{c\pi^N}{\det B} \right)^{3/2} \frac{\gamma^{2K+L} \gamma'^{2K'+L}}{(-c)^{K+K'+L}} \\ \times \sum_{n=0}^{K+K'+L} \frac{1}{(2n+1)!} (-2c)^n \mathcal{F}_V(2n+2, c/2) \\ \times \sum_{k=0}^{\min(K, K')} 4^k B_{kL} H_{n,k}^{K, K', L} \left( \frac{2q\gamma'}{\rho\gamma}, \frac{2q'\gamma'}{\rho\gamma'}, \frac{\rho c}{\gamma\gamma'} \right) \end{aligned} \quad (\text{E9})$$

while, for the special case  $K = K' = 0$ , this formula reduces to [SBM, (C17) page 10]

$$\begin{aligned} \langle \psi_{0LM}(u', A') | V(|\tilde{w}\mathbf{x}|) | \psi_{0LM}(u, A) \rangle = \mathcal{N}_L 2c \sqrt{\frac{c}{2\pi}} L! \\ \times \sum_{n=0}^L \frac{(2c)^n \mathcal{F}_V(2n+2, c/2)}{(2n+1)! (L-n)!} \left( \frac{\gamma\gamma'}{\rho c} \right)^n \left( 1 - \frac{\gamma\gamma'}{\rho c} \right)^{L-n} \end{aligned} \quad (\text{E10})$$

Following the philosophy proposed in SBM, an alternative formula exist for the central matrix elements [SBM, (16) page 3]

$$\begin{aligned} \langle \psi_{K'LM}(u', A') | V(|\tilde{w}\mathbf{x}|) | \psi_{KLM}(u, A) \rangle = \left( \frac{\alpha\pi^N}{\det B} \right)^{\frac{3}{2}} \\ \times \frac{(2K' + L)! (2K + L)!}{B_{K'L} B_{KL}} \sum_{n=0}^{K+K'+L} \left( \frac{\alpha}{2c} \right)^n J(n, \alpha, c) \\ \times \sum_{k=0}^{\min(K, K')} \frac{2^{2k+L}}{(2k+L)!} B_{kL} F_{n,k}^{K, K', L}(\bar{q}, \bar{q}', \gamma, \gamma'). \end{aligned} \quad (\text{E11})$$

which, in the special case  $K = K' = 0$  reduces to [SBM, (21) page 4]

$$\langle \psi_{0LM} | V(|\tilde{w}\mathbf{x}|) | \psi_{0LM} \rangle = \mathcal{N}_L L! \left( \frac{\alpha}{1-\alpha} \right)^L \alpha^{3/2} J(L, \alpha, c). \quad (\text{E12})$$

Using rather the  $\mathcal{F}$  integrals gives another formulation [SBM, (22) page 4]

$$\begin{aligned} \langle \psi_{K'LM}(u', A') | V(|\tilde{w}\mathbf{x}|) | \psi_{KLM}(u, A) \rangle = \\ \frac{4(2K' + L)! (2K + L)!}{\sqrt{\pi} B_{K'L} B_{KL}} \left( \frac{c\pi^N}{2\det B} \right)^{3/2} \\ \times \sum_{n=0}^{K+K'+L} \frac{1}{(2n+1)!} \mathcal{F}_V(2n+2, c/2) \\ \times \sum_{k=0}^{\min(K, K')} \frac{2^{2k+L}}{(2k+L)!} B_{kL} P_{n,k}^{K, K', L}(\bar{q}, \bar{q}', \gamma, \gamma', c), \end{aligned} \quad (\text{E13})$$

while the special case  $K = K' = 0$  gives again the formula (E10) presented before.

Comparing the formulae given in this section with the new ones proposed in the paper shows the tight similarities that exist between all the types of potential.

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